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CONVERGENCE CRITERIA IN NUMERICAL SOLUTION OF THE DIFFUSION EQUATION

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A previous Bureau Circular, AIC-152, is a reprint of a paper first appearing in Chemical Engineering Progress, 43(1):13-24, January 1947, entitled "Approximate Diffusion Calculations for the Falling-Rate Phase of Drying". The procedures described in that paper were based in large part upon a paper by G. M. Dusinberre, Trans. Am. Soc. Mech. Engrs. 67(8):703-712, November 1945. Further study of the application of numerical computation methods to certain problems of drying resulted in a report to the Engineering and Development Division of the Western Regional Research Laboratory concerning criteria for the choice of time increments to be used in the computations. A copy of this report, dated February 14, 1948, and designated ED-6-12-19, was sent to Professor Dusinberre for comments. In 1949 Professor Dusinberre's book, "Numerical Analysis of Heat Flow", appeared. The following reference occurs on pages 201-202:

> "We have developed convergence criteria in a number of forms for transient and quasi-steady states, and these have been based on thermodynamic rather than mathematical reasoning. Fowler [Quart. Appl. Math. 3(4):361-376, Jan. 1946] has applied the methods of contour integration to some of the simple cases and has arrived at criteria which are in no case more restrictive and in some cases less so than those developed here.
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> "Based on perhaps insufficient investigation, we tentatively suggest the following: If Fowler's criterion is exceeded, we definitely get a divergent oscillation. If the two criteria differ, the region between usually leads to a convergent oscillation. The author's criterion usually leads to a monotonic convergence, but sometimes to a convergent oscillation, especially in the first steps of the calculation. Studies of Van Arsdel [reference here to Report ED 6 12 19] tend to support these conclusions.
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> "Van Arsdel [reference here to AIC 152], in the investigation of moisture diffusion in the dehydration of vegetables, has been interested in using the maximum possible values of $\Delta\theta$. This was in order to test as rapidly as possible a large number of hypotheses as to the detailed phenomena involved, which could only be checked by over-all drying rate data. Thus he wished to use limiting values of the criteria

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"His calculation procedure seems equivalent to representing k (in our terminology) as a function of time. A $\Delta\theta$ near the limit was chosen, and when an oscillation began to appear, $\Delta\theta$ was changed. This is typical of the artifices that may be used to adapt the numerical procedure to a particular objective."

Since the publication of Professor Dusinberre's book requests have been received for copies of our report designated ED-6-12-19. The present Bureau Circular is designed to make that previously unpublished report available. The report has been revised only in minor editorial respects.

SUMMARY OF REPORT

Fowler's analysis of convergence results in a criterion which assures a convergent numerical solution, but which applies only to the simplest cases (not, for example, to the non-linear problem). Dusinberre's criterion is applicable to all cases, but has no precise mathematical significance. It is, in general, more restrictive than Fowler's criterion and hence leads to solutions whose oscillation about the true values is strongly damped.

Working formulas based upon Dusinberre's criterion are deduced for the following types of problem:

1. Constant diffusivity, infinite slab, concentration as potential.
2. Variable diffusivity, infinite slab, concentration as potential.
3. Variable diffusivity, infinite slab, moisture content as potential.
4. Variable diffusivity, infinite slab, cylinder, and sphere, moisture content as potential internally, vapor pressure at convective surface.
5. Variable permeability, infinite slab, vapor pressure as potential.

The implications of this analysis for automatic machine calculation are considered briefly.

CONVERGENCE AND OSCILLATION IN NUMERICAL SOLUTIONS

The success of a numerical computation of an unsteady-state diffusion process, using the finite difference method as described by Dusinberre (Trans. A.S.M.E. 67(8): 703-712, Nov. 1945) and others, depends upon such a choice of the finite increments, both of time and of space, that the solution will converge toward "true" values (i.e., those it would take if the increments were infinitesimal in size), and also will be relatively free from oscillation. The latter is ordinarily the more critical consideration, and apparently if it is satisfactorily met, numerical convergence always will be assured as well.

The characteristics of "oscillation" in a solution are more easily described by an actual example than by an abstract definition. Figure 1 pictures data from such an example. The calculated course of moisture content as time increases is shown for two locations in an infinite slab exposed to drying conditions, one location being the surface lamina and the other the lamina next below the surface. The curves designated "$\Delta\theta = \frac{1}{3}$" typify a substantially non-oscillating solution, those designated "$\Delta\theta = 8$" a strongly oscillating solution. In this example the latter curve shows a weakly damped

ALFALFA

Mimeographed Circulars

ALFALFA HAS PROMISING CHEMURGIC FUTURE. AIC-167. July, 1947

ALFALFA--A SELECTED BIBLIOGRAPHY OF ITS COMPOSITION, PROCESSING, AND USE. AIC-24
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FRUIT AND VEGETABLE BYPRODUCTS

Mimeographed Circulars

Subtilin

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